

# Randić Energy and Randić Eigenvalues\*

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## Abstract

Let  $G$  be a graph of order  $n$ , and  $d_i$  the degree of a vertex  $v_i$  of  $G$ . The *Randić matrix*  $\mathbf{R} = (r_{ij})$  of  $G$  is defined by  $r_{ij} = 1/\sqrt{d_j d_i}$  if the vertices  $v_i$  and  $v_j$  are adjacent in  $G$  and  $r_{ij} = 0$  otherwise. The *normalized signless Laplacian matrix*  $\mathcal{Q}$  is defined as  $\mathcal{Q} = I + \mathbf{R}$ , where  $I$  is the identity matrix. The *Randić energy* is the sum of absolute values of the eigenvalues of  $\mathbf{R}$ . In this paper, we find a relation between the normalized signless Laplacian eigenvalues of  $G$  and the Randić energy of its subdivided graph  $S(G)$ . We also give a necessary and sufficient condition for a graph to have exactly  $k$  and distinct Randić eigenvalues.

## 1 Introduction

All graphs considered here are simple, undirected and finite. Let  $G$  be a graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$  and degree sequence  $(d_1, d_2, \dots, d_n)$ , where  $d_i$  is the degree of a vertex  $v_i$  ( $1 \leq i \leq n$ ) of  $G$ . For a graph  $G$ , let  $M = M(G)$  be a corresponding *graph matrix* defined in a prescribed way. The  *$M$ -polynomial* of  $G$  is defined as  $\phi_M(G, \lambda) = \det(\lambda I - M)$ , where  $I$  is the identity matrix. The  *$M$ -eigenvalues* of  $G$  are those of its graph matrix  $M$ . It is well-known that there already exist some graph matrices, including *adjacency matrix*  $A$ , *degree matrix*  $D$ , *Laplacian matrix*  $L = D - A$ , *signless Laplacian matrix*  $Q = D + A$  and so on.

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In 1975, Milan Randić [17] invented a molecular structure descriptor defined as

$$R(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}},$$

where the summation goes over all pairs of adjacent vertices of the underlying (molecular) graph. This graph invariant is nowadays known under the name *Randić index*, for details see [10, 12, 13, 18].

Gutman et al. [11] pointed out that the Randić-index-concept is purposeful to produce a graph matrix of order  $n$ , named *Randić matrix*  $\mathbf{R}(G)$ , whose  $(i, j)$ -entry is defined as

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if } v_i \text{ and } v_j \text{ are adjacent vertices,} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent,} \\ 0 & \text{if } i = j. \end{cases}$$

In what follows, we need the convention that all graphs possess no isolated vertices. Then  $\mathbf{R}(G) = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$ . Recall that the *normalized Laplacian* and *sinless Laplacian matrices* [5] are respectively defined as

$$\mathcal{L}(G) = D^{-\frac{1}{2}} L D^{-\frac{1}{2}} \quad \text{and} \quad \mathcal{Q}(G) = D^{-\frac{1}{2}} Q D^{-\frac{1}{2}}.$$

From this point of view, the eigenvalues of above three matrices have a direct relation. As shown in [11],  $\mathcal{L}(G) = I_n - \mathbf{R}(G)$  and  $\mathcal{Q}(G) = I_n + \mathbf{R}(G)$ . So if an  $\mathbf{R}$ -eigenvalue is  $\rho_i$ , then the  $\mathcal{L}$ -eigenvalue  $\mu_i$  and  $\mathcal{Q}$ -eigenvalue  $\theta_i$  are respectively

$$\mu_i = 1 - \rho_i \quad \text{and} \quad \theta_i = 1 + \rho_i, \quad 1 \leq i \leq n. \quad (1)$$

For the  $\mathcal{L}$ -eigenvalues, there are numerous results; see [5] for example. From Lemmas 1.7–1.8 [5] it follows that  $0 \leq \mu_i \leq 2$ , and so by (1),

$$-1 \leq \rho_i \leq 1 \quad \text{and} \quad 0 \leq \theta_i \leq 2, \quad 1 \leq i \leq n. \quad (2)$$

Gutman [9] introduced the (adjacency) energy of a graph  $G$  as follows

$$E(G) = \sum_{i=1}^n |\lambda_i|,$$

which has been extended to energies of other graph matrices [14, 16]. Especially, the *Randić energy*  $RE(G)$  [1, 2] is defined as

$$RE(G) = \sum_{i=1}^n |\rho_i|.$$

So far, there are quite a few results about the Randić energy and  $\mathbf{R}$ -eigenvalues, which therefore becomes the main research objects of this paper. In the rest of the paper, we will give a relation between the  $\mathcal{Q}$ -eigenvalues of a graph and the Randić energy of its subdivision in Section 2. We also give a necessary and sufficient condition for a graph to have exactly  $k$  and distinct  $R$ -eigenvalues in Section 3, particularly for  $k = 2, 3$ .

## 2 Randić energy and $\mathcal{Q}$ -eigenvalues

Let  $S(G)$  be the subdivision of a graph  $G$  that is obtained by adding a new vertex into each edge of  $G$ . Evidently,  $S(G)$  is a bipartite graph, and so  $V(S(G)) = V_1 \cup V(G)$ , where  $V_1$  is the set of new added vertices of degree two.

The following lemma from matrix theory can be found in, for example, [6] p. 62.

**Lemma 2.1.** *If  $M$  is a nonsingular square matrix, then*

$$\begin{vmatrix} M & N \\ P & F \end{vmatrix} = |M| \cdot |F - PM^{-1}N|.$$

**Lemma 2.2.** *Let  $G$  be a graph with order  $n$  and size  $m$ . Then*

$$\phi_{\mathbf{R}}(S(G), \lambda) = \frac{\lambda^{m-n}}{2^n} \phi_{\mathcal{Q}}(G, 2\lambda^2).$$

**Proof.** Obviously,  $|V(S(G))| = n + m$ . It is well-known that

$$Q = BB^T \quad \text{and} \quad A(S(G)) = \begin{pmatrix} O & B^T \\ B & O \end{pmatrix},$$

where  $B$  is the incident matrix of  $G$  and  $B^T$  is the transpose of  $B$ . Then, we partition the degree matrix  $D(S(G))$  into

$$D(S(G)) = \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix},$$

where  $D_1 = \text{diag}(2, 2, \dots, 2)$  with order  $m \times m$  and  $D_2 = D(G)$ . If  $G$  has no isolated vertices, then so does  $S(G)$ . Consequently,

$$\begin{aligned} \mathbf{R}(S(G)) &= D^{-\frac{1}{2}} A(S(G)) D^{-\frac{1}{2}} = \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} O & B^T \\ B & O \end{pmatrix} \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix} \\ &= \begin{pmatrix} O & D_1^{-\frac{1}{2}} B^T D_2^{-\frac{1}{2}} \\ D_2^{-\frac{1}{2}} B D_1^{-\frac{1}{2}} & O \end{pmatrix}. \end{aligned}$$

By Lemma 2.1 we get

$$\begin{aligned} \phi_{\mathbf{R}}(S(G), \lambda) &= |\lambda I_{m+n} - \mathbf{R}(S(G))| = \begin{vmatrix} \lambda I_m & -D_1^{-\frac{1}{2}} B^T D_2^{-\frac{1}{2}} \\ -D_2^{-\frac{1}{2}} B D_1^{-\frac{1}{2}} & \lambda I_n \end{vmatrix} \\ &= |\lambda I_m| |\lambda I_n - D_2^{-\frac{1}{2}} B D_1^{-\frac{1}{2}} \frac{I_m}{\lambda} D_1^{-\frac{1}{2}} B^T D_2^{-\frac{1}{2}}| \\ &= \lambda^{m-n} |\lambda^2 I_n - \frac{1}{2} D_2^{-\frac{1}{2}} B B^T D_2^{-\frac{1}{2}}| \\ &= \frac{\lambda^{m-n}}{2^n} |2\lambda^2 I_n - \mathcal{Q}| \\ &= \frac{\lambda^{m-n}}{2^n} \phi_{\mathcal{Q}}(G, 2\lambda^2). \end{aligned}$$

This finishes the proof.  $\square$

**Theorem 2.3.** *Let  $G$  be a graph with order  $n$  and size  $m$ .*

- (i) *If  $\phi_{\mathcal{Q}}(G, \lambda) = \sum_{i=0}^n a_i \lambda^{n-i}$ , then  $\phi_{\mathbf{R}}(S(G), \lambda) = \lambda^{m-n} \sum_{i=0}^n 2^{-i} a_i \lambda^{n-i}$ .*
- (ii)  *$\rho$  is an  $\mathbf{R}$ -eigenvalue of  $S(G)$  if and only if  $2\rho^2$  is a  $\mathcal{Q}$ -eigenvalue of  $G$ .*
- (iii) *Let  $\theta_1, \theta_2, \dots, \theta_n$  be the  $\mathcal{Q}$ -eigenvalues of  $G$ . Then  $RE(S(G)) = \sqrt{2} \sum_{i=1}^n \sqrt{\theta_i}$ .*

**Proof.** For (i), by Lemma 2.2 we get

$$\phi_{\mathbf{R}}(S(G), \lambda) = \frac{\lambda^{m-n}}{2^n} \phi_{\mathcal{Q}}(G, 2\lambda^2) = \frac{\lambda^{m-n}}{2^n} \sum_{i=0}^n a_i (\sqrt{2}\lambda)^{2(n-i)} = \lambda^{m-n} \sum_{i=0}^n 2^{-i} a_i \lambda^{n-i}.$$

(ii) is an immediate result of Lemma 2.2. For (iii), from (2) we obtain  $\theta_i \geq 0$ , and so  $\pm\sqrt{\theta_i/2}$  is an  $\mathbf{R}$ -eigenvalue of  $S(G)$  by (i). Thus,  $RE(S(G)) = \sqrt{2} \sum_{i=1}^n \sqrt{\theta_i}$ .  $\square$

**Remark 2.4.** *By Theorem 2.3(i), it becomes easier to compute the Randić energies of some graphs. As an example, Gutman et al. [11] conjectured that the connected graph with odd order and greatest Randić energy is the sun, which is exactly the subdivision of the star  $S_n$ . Easy to compute  $\phi_{\mathcal{Q}}(S_n, \theta) = \theta(\theta - 1)^{n-2}(\theta - 2)$ . Hence,  $RE(S(S_n)) = \sqrt{2}n + 2 - 2\sqrt{2}$ .*

### 3 Connected graphs with distinct $\mathbf{R}$ -eigenvalues

A popular and important research field is to investigate the connected graphs with distinct eigenvalues. As van Dam said, it is an interplay between combinatorics and algebra; for details see his thesis [7]. Inspired by his ideas, we give a necessary and sufficient condition for a graph to have  $k$  distinct  $\mathbf{R}$ -eigenvalues.

It has been proved that  $\rho_1 = 1$  is the largest  $\mathbf{R}$ -eigenvalues with the Perron-Frobenius vector  $\alpha^T = (\sqrt{d_1}, \sqrt{d_2}, \dots, \sqrt{d_n})$ ; see [4, 11, 15].

**Theorem 3.1.** *Let  $G$  be connected graph with order  $n \geq 3$  and size  $m$ . Then  $G$  has exactly  $k$  ( $2 \leq k \leq n$ ) and distinct  $\mathbf{R}$ -eigenvalues if and only if there are  $k - 1$  distinct none-one real numbers  $\rho_2, \rho_3, \dots, \rho_k$  satisfying*

$$\prod_{i=2}^k (\mathbf{R} - \rho_i I) = \frac{\prod_{i=2}^k (1 - \rho_i)}{2m} \alpha \alpha^T. \quad (3)$$

*Moreover,  $1, \rho_2, \dots, \rho_k$  are exactly the  $k$  distinct  $\mathbf{R}$ -eigenvalues of  $G$ .*

**Proof.** Let  $\rho_1 = 1, \rho_2, \rho_3, \dots, \rho_k$  be the  $k$  distinct  $\mathbf{R}$ -eigenvalues. Since  $\mathbf{R}$  is a real symmetric matrix, it must be diagonalizable, and thus the minimal polynomial of  $\mathbf{R}$  is  $(\lambda - \rho_1)(\lambda - \rho_2) \cdots (\lambda - \rho_k)$ . Hence,

$$\Pi_{i=1}^n (\mathbf{R} - \rho_i I) = O, \quad \text{that is,} \quad (\mathbf{R} - \rho_1 I)(\Pi_{i=2}^n (\mathbf{R} - \rho_i I)) = O.$$

Since  $G$  is connected, by Perron-Frobenius Theorem we know that the algebraic multiplicity of  $\rho_1 = 1$  is one, and so is the geometric multiplicity. Consequently, each column of  $H = \prod_{i=2}^n (\mathbf{R} - \rho_i I) = (h_1, h_2, \dots, h_n)$  is a scalar multiple of the Perron-Frobenius vector  $\alpha$ . Set  $h_i = a_i \alpha$  ( $1 \leq i \leq n$ ). So,  $H = \alpha(a_1, a_2, \dots, a_n)$  and thus

$$\alpha^T H = \alpha^T \alpha (a_1, a_2, \dots, a_n).$$

By a direct calculation we have

$$\prod_{i=2}^k (1 - \rho_i) \alpha^T = 2m(a_1, a_2, \dots, a_n),$$

leading to

$$a_i = \frac{\prod_{i=2}^k (1 - \rho_i)}{2m} \sqrt{d_i} \quad (i = 1, 2, \dots, k).$$

The necessity thus follows.

For the sufficiency, multiplying  $\mathbf{R} - \rho_1 I$  ( $\rho_1 = 1$ ) to both sides of (3), we arrive at

$$(\mathbf{R} - \rho_1 I) \prod_{i=2}^k (\mathbf{R} - \rho_i I) = \frac{\prod_{i=2}^k (1 - \rho_i)}{2m} ((\mathbf{R} - I) \alpha) \alpha^T = O.$$

So,  $m(x) = (x - \rho_1)(x - \rho_2) \cdots (x - \rho_k)$  is an annihilating polynomial of  $\mathbf{R}$ , i.e., a polynomial with value at  $\mathbf{R}$  is a 0-matrix. From (3) follows  $\prod_{i=2}^k (\mathbf{R} - \rho_i I) \neq O$ , which shows that the product of some factors taken from  $\{x - \rho_2, \dots, x - \rho_k\}$  is not a minimal polynomial of  $\mathbf{R}$ . Hence,  $m(x)$  is the minimal polynomial, and thus  $1, \rho_2, \dots, \rho_k$  are the  $k$  distinct  $\mathbf{R}$ -eigenvalues.  $\square$

Bozkurt et al. [2] determined the connected graphs with two distinct  $\mathbf{R}$ -eigenvalues. We now give another short proof based on the above theorem.

**Corollary 3.2.** *A connected graph  $G$  has exactly two and distinct  $\mathbf{R}$ -eigenvalues if and only if  $G$  is a complete graph.*

**Proof.** It is known that the complete graph of order  $n$  has exactly two distinct  $\mathbf{R}$ -eigenvalues 1 and  $-\frac{1}{n-1}$  [6]. Substituting 1 and  $-\frac{1}{n-1}$  into Eq. (3) we get

$$\mathbf{R}(G) = \frac{1}{(n-1)^2} \alpha \alpha^T - \frac{1}{n-1} I.$$

Considering the diagonal entries in both sides of the above equality, we have

$$\frac{1}{(n-1)^2} d_i - \frac{1}{n-1} = 0,$$

and so  $d_i = n - 1$  ( $i = 1, 2, \dots, n$ ). Hence,  $G$  is a complete graph.  $\square$

For the graph with exactly three and distinct  $\mathbf{R}$ -eigenvalues, the following characterization is given. We denote the number of common neighbors by  $\delta_{ij}$  if vertices  $v_i$  and  $v_j$  are adjacent, and by  $\sigma_{ij}$  if they are not.

**Corollary 3.3.** *Let  $c = \frac{\prod_{i=2}^k (1-\rho_i)}{2m}$ . A connected graph  $G$  has exactly three and distinct  $\mathbf{R}$ -eigenvalues  $1, \rho_2, \rho_3$  if and only if the following items hold:*

- (i) *for any vertex  $u_i$ ,  $\sum_{v_j \sim u_i} \frac{1}{d_j} = cd_i^2 - \rho_2 \rho_3 d_i$ ,*
- (ii) *for adjacent vertices  $u_i$  and  $v_j$ ,  $\delta_{ij} = cd_i d_j + \rho_2 + \rho_3$ ,*
- (iii) *for nonadjacent vertices  $u_i$  and  $v_j$ ,  $\sigma_{ij} = cd_i d_j$ .*

**Proof.** From Theorem 3.1 we get  $(\mathbf{R} - \rho_2 I)(\mathbf{R} - \rho_3 I) = c\alpha\alpha^T$ . Then the results follow by considering the diagonal entries and nondiagonal entries for both sides of this equality.  $\square$

Note that a  $k$ -regular graph of order  $n$  ( $0 < k < n - 1$ ) is *strong regular* with parameters  $(n, k, \delta, \sigma)$  if the number of common neighbors of any two distinct vertices equals  $\delta$  if the vertices are adjacent and  $\sigma$  otherwise [3]. The following result follows from Corollary 3.3.

**Corollary 3.4.** *A regular connected graph has exactly three and distinct  $\mathbf{R}$ -eigenvalues if and only if it is strong regular.*

From (1) it follows that a connected graph has exactly  $k$  distinct  $\mathbf{R}$ -eigenvalues if and only if it has  $k$  distinct  $\mathcal{L}$ -ones. van Dam and Omid  $\text{\AA}$  [8] found such graphs and pointed out that a complete classification of such graphs still seems out of reach. In subsequent work, it seems interesting to determine connected graphs with exactly four or more and distinct  $\mathbf{R}$ -eigenvalues. Furthermore, due to  $\mathcal{L} = I - \mathbf{R}$ , it seems much simpler to investigate on this topic by the  $\mathbf{R}$ -eigenvalues.

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